## Biotinylation of a MRI/Gd BNCT Theranostic Agent to Access a Novel Tumor-Targeted Delivery System

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Spectral characterization of products 3, 4, 5, 6, 8, 9, 12, 13, 14, 15, 17, AL01\_\_\_\_\_\_pag. 2-49EC50 (half maximal effective concentration) of Gd-AL01\_\_\_\_\_\_pag. 50



<sup>1</sup>H NMR of compound **4** (600 MHz, CDCl<sub>3</sub>)





<sup>13</sup>C NMR of compound **4** (150 MHz, CDCl<sub>3</sub>)





Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **4** (150 MHz, CDCl3)



<sup>13</sup>C NMR of compound **5** (150 MHz, CDCl<sub>3</sub>)











<sup>13</sup>C NMR of compound **6** (150 MHz, CDCl<sub>3</sub>)



Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **6** (150 MHz, CDCl<sub>3</sub>)









<sup>13</sup>C NMR of compound **8** (150 MHz, CDCl<sub>3</sub>)





Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **8** (150 MHz, CDCl<sub>3</sub>)

<sup>11</sup>B NMR of compound **8** (192.5 MHz, CDCl<sub>3</sub>)



Deconvolution (left), spectrum generated after deconvolution of <sup>11</sup>B NMR of compound **8** (right)























## Deconvolution (left), spectrum generated after deconvolution of <sup>11</sup>B NMR of compound **9** (right)



<sup>1</sup>H NMR of compound **12** (600 MHz, CDCl<sub>3</sub>)





<sup>13</sup>C NMR of compound **12** (150 MHz, CDCl<sub>3</sub>)

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Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **12** (150 MHz, CDCl<sub>3</sub>)



<sup>1</sup>H NMR of compound **13** (600 MHz, DMSO-d<sup>6</sup>)



<sup>1</sup>H NMR of compound **14** (600 MHz, MeOD)





COSY <sup>1</sup>H NMR of compound **14** (600 MHz, MeOD)

<sup>13</sup>C NMR of compound **14** (150 MHz, MeOD)





Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **14** (150 MHz, MeOD)



Deconvolution (left), spectrum generated after deconvolution of <sup>11</sup>B NMR of compound **14** (right)





<sup>1</sup>H NMR of compound **15** (600 MHz, MeOD)









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Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **15** (150 MHz, MeOD)

<sup>11</sup>B NMR of compound **15** (192.5 MHz, MeOD)



Deconvolution (left), spectrum generated after deconvolution of <sup>11</sup>B NMR of compound **15** (right)



<sup>1</sup>H NMR of compound **17** (600 MHz, MeOD)





COSY <sup>1</sup>H NMR of compound **17** (600 MHz, MeOD)

<sup>13</sup>C NMR of compound **17** (150 MHz, MeOD)



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Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **17** (150 MHz, MeOD)

<sup>11</sup>B NMR of compound **17** (192.5 MHz, MeOD)



Deconvolution (left), spectrum generated after deconvolution <sup>11</sup>B NMR of compound **17** (right)







COSY <sup>1</sup>H NMR of compound AL101 (600 MHz, MeOD)

<sup>13</sup>C NMR of compound AL101 (150 MHz, MeOD)





Comparison between DEPT-135 and <sup>13</sup>C NMR of compound **AL101** (150 MHz, MeOD)





Deconvolution (left), spectrum generated after deconvolution <sup>11</sup>B NMR of compound **AL101** (right)



Dose-response curve (in MTT assay) on HeLa cells and on NIH/3T3 for Gd-AL01 incubated for 24h in a concentration range 0.0016-0.57 mM.



The EC50 (half maximal effective concentration) of Gd-AL01 obtained by the dose-response curves after 24h incubation in cell medium was 0.387mM and 0.583mM for HeLa and NIH/3T3, respectively.